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Stereospecificity in the proton magnetic relaxation rate of enantiotopic methyls and the methyl rotation barrier

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Abstract

It is proposed that a distinction should be made between stereospecificity of the first kind, which provides spectral (line assignments in the NMR spectrum) and structural (molecular conformations) information, and stereospecificity of the second kind, which only provides spectral information, on the basis of the relaxation times T1. The nature of the stereospecificity was revealed in detail during analysis of the reasons for the differences in the proton relaxation times of enantiotopic gem-dimethyl groups in the conformationally rigid molecule of 2-oxo-5-5-dimethyl-1,3,2-dioxathiane. It is suggested that the barrier to rotation of the methyl in the geminal CH3-C-H fragment can be assessed from the temperature dependence of the t1 time of the methine proton. The experiment was carried out with the stereoisomeric r-2-tert-but-l-4-methyl-trans-7-methyl[2]1,3-dioxepane. © 1987 Plenum Publishing Corporation.

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